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Gaussian quadrature for multiple orthogonal polynomials[☆]

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Abstract

We study multiple orthogonal polynomials of type I and type II, which have orthogonality conditions with respect to r measures. These polynomials are connected by their recurrence relation of order $r + 1$. First we show a relation with the eigenvalue problem of a banded lower Hessenberg matrix L_n , containing the recurrence coefficients. As a consequence, we easily find that the multiple orthogonal polynomials of type I and type II satisfy a generalized Christoffel–Darboux identity. Furthermore, we explain the notion of multiple Gaussian quadrature (for proper multi-indices), which is an extension of the theory of Gaussian quadrature for orthogonal polynomials and was introduced by Borges. In particular, we show that the quadrature points and quadrature weights can be expressed in terms of the eigenvalue problem of L_n .

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1. Introduction

Multiple orthogonal polynomials arise naturally in the theory of simultaneous rational approximation, in particular in the Hermite–Padé approximation of a system of $r \in \mathbb{N}$ (Markov and Stieltjes) functions [7,8,15,16]. They are a generalization of orthogonal polynomials in the sense that they satisfy orthogonality conditions with respect to measures μ_1, \dots, μ_r ($r \in \mathbb{N}$), for which all the moments exist. In the

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literature one can find already many examples of such polynomials [1–4,18]. Normally measures are taken to be positive. However, in this paper we study *formal* multiple orthogonal polynomials which means that we allow complex measures.

We will only consider multiple orthogonal polynomials with respect to *proper multi-indices*. The proper multi-index corresponding to $n \in \mathbb{N}_0 = \mathbb{N} \cup \{0\}$ is

$$\vec{v}_n = \left(\underbrace{m+1, m+1, \dots, m+1}_{s \text{ times}}, \underbrace{m, m, \dots, m}_{r-s \text{ times}} \right) \in \mathbb{N}_0^r,$$

where $n = mr + s$, $0 < s \leq r$. There exist two types of multiple orthogonal polynomials, type I and type II. Let $\Gamma_1, \dots, \Gamma_r$ be the supports of the r measures. A multiple orthogonal polynomial $P_n = P_{\vec{v}_n}$ of type II with respect to the proper multi-index \vec{v}_n , is a polynomial of degree at most n , which satisfies the orthogonality conditions

$$\int_{\Gamma_j} P_n(x) x^\ell d\mu_j(x) = 0, \quad \ell = 0, \dots, \vec{v}_n(j) - 1, \quad j = 1, \dots, r. \quad (1.1)$$

Here $\vec{v}_n(j)$ is the j th component of \vec{v}_n . Eq. (1.1) leads to a system of n homogeneous linear equations for the $n+1$ unknown coefficients of P_n . A basic requirement to have a good definition is that every possible solution of the system (1.1) has exactly degree n . This is equal to the assumption that (1.1) has a unique solution (up to a scalar multiplicative constant) which has exactly degree n . In that case we call \vec{v}_n a *normal multi-index* for μ_1, \dots, μ_r . Let $m_\ell^{(j)} = \int_{\Gamma_j} x^\ell d\mu_j(x)$ be the ℓ th moment of the measure μ_j and set

$$D_n = (D_{n, \vec{v}_n(1)}^{(1)} \cdots D_{n, \vec{v}_n(r)}^{(r)})^T, \quad (1.2)$$

where

$$D_{n, \ell}^{(j)} = \begin{pmatrix} m_0^{(j)} & m_1^{(j)} & \cdots & m_{\ell-1}^{(j)} \\ m_1^{(j)} & m_2^{(j)} & \cdots & m_\ell^{(j)} \\ \vdots & \vdots & & \vdots \\ m_{n-1}^{(j)} & m_n^{(j)} & \cdots & m_{n+\ell-2}^{(j)} \end{pmatrix}$$

is an $n \times \ell$ matrix of moments of the measure μ_j . Then D_n is the matrix of the linear system (1.1), without the last column. It is known and easily verified that \vec{v}_n is normal if and only if D_n has rank n [3,4,16]. In the case that all the proper multi-indices \vec{v}_n , $n \in \mathbb{N}$, are normal, we call the system of measures a *weakly complete system*.

A type I multiple orthogonal vector polynomial $\vec{A}_n = \vec{A}_{\vec{v}_n} = (A_{n,1}, \dots, A_{n,r})^T$, corresponding to the proper multi-index \vec{v}_n , consists of r polynomials $A_{n,j}$ of degree at most $\vec{v}_n(j) - 1$, satisfying the orthogonality conditions

$$\int x^\ell \sum_{j=1}^r A_{n,j}(x) d\mu_j(x) = 0, \quad \ell = 0, 1, \dots, n-2. \quad (1.3)$$

The usual requirement is that every $A_{n,j}$ has exactly degree $\vec{v}_n(j) - 1$. However, as mentioned before, in this paper we only consider proper multi-indices. So, if the system (1.3) has a unique solution up to a

multiplicative scalar constant and $A_{n,s}$ has exactly degree m , where $n = mr + s$, $0 < s \leq r$, we obtain a good definition. Note that these conditions are satisfied if \vec{v}_{n-1} is normal, which means that D_{n-1} has rank $n - 1$. This easily follows from the fact that the matrix of the linear system (1.3), without the $s(m + 1)$ th column, is equal to D_{n-1}^T .

In Section 3 we approximate integrals of the kind

$$\int_{\Gamma_j} f(x) d\mu_j(x), \quad j = 1, \dots, r,$$

simultaneously, using weighted quadrature formulas which have the same n quadrature nodes. This was already studied by Borges in [5] and by Fidalgo Prieto et al. in [10]. The point of interest then is to find the appropriate quadrature nodes and weights maximizing the vector order of the weighted quadrature formulas along the proper multi-indices. In [5, Theorem 2], Borges showed that this is obtained if we require each weighted quadrature formula to be interpolating and the quadrature nodes to be the zeros of the type II multiple orthogonal polynomial P_n , assumed to be simple. We recall this notion of *multiple Gaussian quadrature* in Theorem 3.1.

In the case of Gaussian quadrature ($r = 1$) the nodes and weights can be expressed in terms of the eigenvalue problem of a Jacobi matrix, containing the recurrence coefficients; see, e.g. [11, Chapter 3, Section 2.3]; [12]. In Theorem 3.2 we extend this to multiple Gaussian quadrature. Here we need some properties of multiple orthogonal polynomials. In Section 2 we recall that, for a weakly complete system, the multiple orthogonal polynomials of type I and type II each satisfy a recurrence relation of order $r + 1$ which are closely connected; see, e.g., [15, Section 24]; [6,13,17,19]. As a consequence, these polynomials of type I and type II are then linked to the left and right eigenvalue problem, respectively, of a banded lower Hessenberg matrix L_n containing the recurrence coefficients as in (2.8). This then also leads to a generalized Christoffel–Darboux identity in Theorem 2.5, similar to [17, (21)]. Using all this, we show that in the case of multiple Gaussian quadrature the nodes are the eigenvalues of L_n and the weights can be expressed in terms of the corresponding left and right eigenvectors.

2. Recurrence relation of order $r + 1$

2.1. Relation between type I and type II

Suppose that the system of measures μ_1, \dots, μ_r forms a weakly complete system. The monic multiple orthogonal polynomials P_n of type II corresponding to proper multi-indices are then uniquely determined. Furthermore, as mentioned in the introduction also, the multiple orthogonal polynomials of type I, \tilde{A}_n , are unique up to a normalizing multiplicative constant. In this paper we take the normalization

$$\int x^{n-1} \sum_{j=1}^r A_{n,j}(x) d\mu_j(x) = 1. \quad (2.1)$$

Note that the integral in (2.1) cannot be zero since \vec{v}_n is a normal multi-index.

It is known that multiple orthogonal polynomials satisfy a recurrence relation of order $r + 1$; see, e.g., [14, Section 24; 6, 12, 16, 18]. For the monic multiple orthogonal polynomials of type II this is

$$x P_n(x) = P_{n+1}(x) + \sum_{j=0}^r a_{n,j} P_{n-j}(x), \quad n \geq 0, \quad (2.2)$$

with initial conditions $P_0 \equiv 1$ and $P_j \equiv 0$, $j = -1, -2, \dots, -r$. The proof is similar to that in the case of orthogonal polynomials. Furthermore, there exist some integral representations for the recurrence coefficients in terms of the multiple orthogonal polynomials of type I and type II. If we integrate (2.2) with respect to measures $\sum_{\ell=1}^r A_{n+1-k,\ell}(x) d\mu_\ell(x)$, $k = 0, 1, \dots, r$, then we find

$$\begin{aligned} \int x P_n(x) \sum_{\ell=1}^r A_{n+1-k,\ell}(x) d\mu_\ell(x) &= \int P_{n+1}(x) \sum_{\ell=1}^r A_{n+1-k,\ell}(x) d\mu_\ell(x) \\ &\quad + \sum_{j=0}^r a_{n,j} \int P_{n-j}(x) \sum_{\ell=1}^r A_{n+1-k,\ell}(x) d\mu_\ell(x). \end{aligned}$$

Now apply the orthogonality relations of the multiple orthogonal polynomials of type I and type II. Because of the normalization (2.1) and the fact that the P_n are monic, we then obtain

$$a_{n,j} = \int x P_n(x) \sum_{\ell=1}^r A_{n+1-j,\ell}(x) d\mu_\ell(x), \quad j = 0, 1, \dots, \min(r, n). \quad (2.3)$$

The multiple orthogonal polynomials of type I also satisfy a recurrence relation of order $r + 1$ which is related to the one of type II. Denote by $\mathbb{C}^r[x]$ the space of r -dimensional vector polynomials with complex coefficients. The vector polynomials \vec{A}_n then form a basis for $\mathbb{C}^r[x]$, so that there exist unique $c_{n,k} \in \mathbb{C}$ for which $x \vec{A}_n(x) = \sum_{k=1}^{n+r} c_{n,k} \vec{A}_k(x)$. By linearity we then have

$$\int x P_i(x) \sum_{\ell=1}^r A_{n,\ell}(x) d\mu_\ell(x) = \sum_{k=1}^{n+r} c_{n,k} \int P_i(x) \sum_{\ell=1}^r A_{k,\ell}(x) d\mu_\ell(x), \quad i = 0, 1, \dots$$

The cases $i = 0, 1, \dots, n - 3$ give rise to $c_{n,1} = \dots = c_{n,n-2} = 0$ by the orthogonality relations (1.3). Furthermore, use the orthogonality relations (1.1) and the normalization (2.1) to get

$$c_{n,n-1} = 1, \quad c_{n,n+j} = \int x P_{n+j-1}(x) \sum_{\ell=1}^r A_{n,\ell}(x) d\mu_\ell(x), \quad j = 0, 1, \dots, r.$$

Comparing this with (2.3) we obtain $c_{n,n+j} = a_{n+j-1,j}$, $j = 0, 1, \dots, r$. So if the monic multiple orthogonal polynomials of type II satisfy the recurrence relation (2.2) then the multiple orthogonal polynomials of

type I with normalization (2.1) satisfy the recurrence relation

$$x \vec{A}_n(x) = \vec{A}_{n-1}(x) + \sum_{j=0}^r a_{n+j-1,j} \vec{A}_{n+j}(x), \quad n \geq 1, \quad (2.4)$$

with initial conditions $\vec{A}_0 \equiv \vec{0}$ and $\vec{A}_1, \dots, \vec{A}_r$. Denote by $D_n^{(j,i)}$ the matrix obtained from D_n by deleting the j th row and the i th column (and set $\det D_1^{(1,1)}$ equal to 1). For $1 \leq i, j \leq r$ we then have

$$A_{i,j} = \begin{cases} (-1)^{i+j} \frac{\det D_i^{(j,i)}}{\det D_i}, & j \leq i, \\ 0, & j > i, \end{cases} \quad (2.5)$$

which are functions of the (first r) moments of the measures μ_1, \dots, μ_r . Notice that $A_{j,j} \neq 0, j = 1, \dots, r$, because the multi-indices \vec{v}_n are normal.

Remark 2.1. Let $n = mr + s, 0 < s \leq r$. Applying the orthogonality conditions of the polynomial P_{n+r-1} , we obtain from (2.3)

$$\begin{aligned} a_{n+r-1,r} &= \int x P_{n+r-1}(x) \sum_{\ell=1}^r A_{n,\ell}(x) d\mu_\ell(x) \\ &= \int x P_{n+r-1}(x) A_{n,s}(x) d\mu_s(x), \quad n \geq 1. \end{aligned}$$

We assumed that \vec{v}_{n-1} and \vec{v}_{n+r} are normal, so $A_{n,s}$ has exactly degree m and

$$a_{n+r-1,r} \neq 0, \quad n \geq 1. \quad (2.6)$$

This means that we can recover the vector polynomials \vec{A}_n by (2.4) if we know the initial conditions (2.5) and the recurrence coefficients.

Remark 2.2. We supposed that the measures μ_1, \dots, μ_r form a weakly complete system. If we replace these measures by

$$\alpha_{1,1}\mu_1, \alpha_{2,1}\mu_1 + \alpha_{2,2}\mu_2, \dots, \sum_{j=1}^r \alpha_{r,j}\mu_j, \quad (2.7)$$

where $\alpha_{i,j} \in \mathbb{C}, 1 \leq j \leq i \leq r$, then it is clear that this system of measures forms a weakly complete system if and only if $\alpha_{j,j} \neq 0, j = 1, \dots, r$. Furthermore, all these systems of measures have the same multiple orthogonal polynomials of type II with proper multi-indices and so the same recurrence coefficients. It is obvious that every set of measures of form (2.7) then corresponds to another choice of initial conditions for the recurrence relation (2.4) where $A_{j,j} \neq 0, j = 1, \dots, r$.

2.2. Eigenvalue problem of the banded Hessenberg matrix L_n

In this section, we introduce the banded lower Hessenberg matrix

$$L_n = \begin{pmatrix} a_{0,0} & 1 & 0 & \dots & \dots & \dots & \dots & \dots & 0 \\ a_{1,1} & a_{1,0} & 1 & 0 & & & & & 0 \\ a_{2,2} & a_{2,1} & a_{2,0} & 1 & 0 & & & & 0 \\ \vdots & & \ddots & \ddots & \ddots & \ddots & & & \vdots \\ a_{r,r} & \dots & \dots & a_{r,1} & a_{r,0} & 1 & 0 & & 0 \\ 0 & a_{r+1,r} & \dots & \dots & a_{r+1,1} & a_{r+1,0} & 1 & 0 & 0 \\ \vdots & \ddots & \ddots & & & \ddots & \ddots & \ddots & \vdots \\ \vdots & & \ddots & \ddots & & & \ddots & \ddots & 0 \\ \vdots & & & \ddots & \ddots & & & \ddots & 1 \\ 0 & \dots & \dots & \dots & 0 & a_{n-1,r} & \dots & \dots & a_{n-1,1} & a_{n-1,0} \end{pmatrix}, \quad (2.8)$$

which contains the recurrence coefficients of the multiple orthogonal polynomials. If we expand the determinant $\det(xI_n - L_n)$ along the last row, then we find that these polynomials satisfy the recurrence relation (2.2). So $P_n(x) = \det(xI_n - L_n)$ and the eigenvalues $x_{1,n}, \dots, x_{n,n}$ of the matrix L_n then coincide with the zeros of the polynomial P_n . We now have a closer look at the relation between the type I and type II multiple orthogonal polynomials and the eigenvectors of L_n . The first n relations of the recurrence (2.2) can be written as

$$L_n \begin{pmatrix} P_0(x) \\ \vdots \\ P_{n-2}(x) \\ P_{n-1}(x) \end{pmatrix} + \begin{pmatrix} 0 \\ \vdots \\ 0 \\ P_n(x) \end{pmatrix} = x \begin{pmatrix} P_0(x) \\ \vdots \\ P_{n-2}(x) \\ P_{n-1}(x) \end{pmatrix}. \quad (2.9)$$

Substituting $x = x_{\ell,n}$, $\ell = 1, \dots, n$, we then conclude that $(P_0(x_{\ell,n}) \cdots P_{n-1}(x_{\ell,n}))^T$ is the (only possible) right eigenvector of L_n corresponding to the eigenvalue $x_{\ell,n}$, normalized so that the first component is equal to 1. Note that the first component of a right eigenvector of L_n cannot be 0, otherwise each component would be 0.

For the type I polynomials we can find something similar. Define for $i = 1, \dots, r$ the vector polynomials

$$\vec{B}_n^{(i)}(x) = x \vec{A}_{n-i+1}(x) - \vec{A}_{n-i}(x) - \sum_{j=0}^{i-1} a_{n+j-i,j} \vec{A}_{n-i+j+1}(x), \quad (2.10)$$

$$= \sum_{j=i}^r a_{n-i+j,j} \vec{A}_{n-i+j+1}(x), \quad (2.11)$$

where we use definition (2.11), with $a_{\ell_1, \ell_2} = 1$, $0 \leq \ell_1 < \ell_2 \leq r$, in the cases $1 \leq n < i \leq r$. The first n relations of the recurrence (2.4) then are

$$(\vec{A}_1(x) \cdots \vec{A}_n(x))L_n + \left(\underbrace{\vec{0} \cdots \vec{0}}_{n-r^*} \vec{B}_n^{(r^*)}(x) \cdots \vec{B}_n^{(1)}(x) \right) = x(\vec{A}_1(x) \cdots \vec{A}_n(x)), \quad (2.12)$$

where $r^* = \min(r, n)$.

Definition 2.3. Construct the polynomials $\vec{B}_n^{(i)}$, $i = 1, \dots, r$, as in (2.10) and define for $n \in \mathbb{N}$ and $i = 1, \dots, \min(r, n)$ the polynomials

$$Q_{k,n}^{(i)}(x) = \det(\vec{B}_n^{(1)}(x) \cdots \vec{B}_n^{(i-1)}(x) \vec{A}_k(x) \vec{B}_n^{(i+1)}(x) \cdots \vec{B}_n^{(r)}(x)), \quad (2.13)$$

$k \in \mathbb{N}$. We also define

$$B_n(x) = \det(\vec{B}_n^{(1)}(x) \cdots \vec{B}_n^{(r)}(x)), \quad n \in \mathbb{N}. \quad (2.14)$$

Note that each linear combination of the components of the vector polynomials \vec{A}_k satisfies a similar relation as in (2.12). In particular, for the polynomials $Q_{k,n}^{(i)}$, $i = 1, \dots, \min(r, n)$, we get

$$(Q_{1,n}^{(i)}(x) \cdots Q_{n,n}^{(i)}(x))L_n + B_n(x)\vec{e}_{n-i+1}^T = x(Q_{1,n}^{(i)}(x) \cdots Q_{n,n}^{(i)}(x)), \quad (2.15)$$

where \vec{e}_ℓ , $1 \leq \ell \leq n$, is the ℓ th unit vector in \mathbb{R}^n . In Lemma 2.4 below we will prove that the polynomial B_n is equal to P_n up to a multiplicative nonzero constant. Eq. (2.15) then implies that the vectors

$$(Q_{1,n}^{(i)}(x_{\ell,n}) \cdots Q_{n,n}^{(i)}(x_{\ell,n}))^T, \quad i = 1, \dots, \min(r, n), \quad (2.16)$$

are left eigenvectors of the matrix L_n corresponding to the eigenvalue $x_{\ell,n}$, if they are different from $\vec{0}$.

Lemma 2.4. Let \vec{A}_n the vector polynomials defined by the recurrence relation (2.4) and its initial conditions (with $A_{j,j} \neq 0$, $j = 1, \dots, r$). Here we assume that the recurrence coefficients $a_{\ell,r}$, $\ell \geq r$, are different from 0. For the polynomials B_n we then have that $B_n(x) = \gamma_n P_n(x)$, where the P_n are the monic polynomials defined by the recurrence relation (2.2) and

$$\gamma_n = \frac{\prod_{j=1}^r A_{j,j}}{\prod_{\ell=r}^{n-1} a_{\ell,r}} (-1)^{\lfloor \frac{s}{2} \rfloor + \lfloor \frac{r-s}{2} \rfloor}, \quad n = mr + s, \quad 0 < s \leq r. \quad (2.17)$$

Proof. First of all we prove that B_n is a polynomial of exactly degree n with leading coefficient γ_n . Using (2.11) we find that

$$\begin{aligned} B_n(x) &= \det(\vec{B}_n^{(1)}(x) \cdots \vec{B}_n^{(r)}(x)) \\ &= \prod_{\ell=n}^{n+r-1} a_{\ell,r} \det(\vec{A}_{n+r}(x) \cdots \vec{A}_{n+1}(x)) \end{aligned} \quad (2.18)$$

$$= \prod_{\ell=n}^{n+r-1} a_{\ell,r} \sum_{\pi \in S_r} \text{sign}(\pi) A_{n+r,\pi(1)}(x) \cdots A_{n+1,\pi(r)}(x), \quad (2.19)$$

where we denote by S_r the set of permutations of r elements. Note that from the recurrence relation (2.4) and its initial conditions, with $A_{j,j} \neq 0$, $j = 1, \dots, r$ and $a_{\ell,r} \neq 0$, $\ell \geq r$, we obtain that

$$A_{mr+s,s}(x) = \frac{A_{s,s}}{\prod_{i=1}^m a_{ir+s-1,r}} x^m + \mathcal{O}(x^{m-1}), \quad 1 \leq s \leq r, \quad m \in \mathbb{N} \cup \{0\}. \quad (2.20)$$

Combining this and (2.19) we see that, with $n = mr + s$, $0 < s \leq r$,

$$\deg(B_n(x)) = \deg \left(\underbrace{A_{n+r,s}(x) \cdots A_{n+r-s+1,1}(x)}_s \underbrace{A_{n+r-s,r}(x) \cdots A_{n+1,s+1}(x)}_{r-s} \right) = n,$$

where we note that all the other terms in (2.19) have lower degree. The sign of the permutation corresponding to this term is $(-1)^{\lfloor s/2 \rfloor + \lfloor (r-s)/2 \rfloor}$ so that γ_n is the leading coefficient of B_n .

To complete the proof we show that the polynomials B_n/γ_n satisfy the recurrence relation (2.2). Note that

$$\frac{\gamma_n}{\gamma_{n-j}} = \frac{(-1)^{(r-1)j}}{\prod_{\ell=n-j}^{n-1} a_{\ell,r}}, \quad 1 \leq j \leq n, \quad (2.21)$$

where we assume $a_{0,r} = \cdots = a_{r-1,r} = 1$. By (2.21) and (2.18), we then obtain that

$$\begin{aligned} &\gamma_n \left(\frac{B_{n+1}(x)}{\gamma_{n+1}} + (a_{n,0} - x) \frac{B_n(x)}{\gamma_n} + \sum_{j=1}^r a_{n,j} \frac{B_{n-j}(x)}{\gamma_{n-j}} \right) \\ &= (-1)^{r-1} a_{n,r} B_{n+1}(x) + (a_{n,0} - x) B_n(x) + \sum_{j=1}^r (-1)^{(r-1)j} a_{n,j} \frac{B_{n-j}(x)}{\prod_{\ell=n-j}^{n-1} a_{\ell,r}}, \\ &= (-1)^{r-1} \prod_{\ell=n}^{n+r} a_{\ell,r} \det(\vec{A}_{n+r+1}(x) \cdots \vec{A}_{n+2}(x)) \\ &\quad + (a_{n,0} - x) \prod_{\ell=n}^{n+r-1} a_{\ell,r} \det(\vec{A}_{n+r}(x) \cdots \vec{A}_{n+1}(x)) \\ &\quad + \sum_{j=1}^r (-1)^{(r-1)j} a_{n,j} \prod_{\ell=n}^{n-j+r-1} a_{\ell,r} \det(\vec{A}_{n-j+r}(x) \cdots \vec{A}_{n-j+1}(x)). \end{aligned} \quad (2.22)$$

From the recurrence relation (2.4) we first of all get that

$$\begin{aligned} & (-1)^{r-1} a_{n+r,r} \det(\vec{A}_{n+r+1}(x) \cdots \vec{A}_{n+2}(x)) \\ &= (-1)^{r-1} \det(-\vec{A}_n(x) - (a_{n,0} - x) \vec{A}_{n+1}(x) \vec{A}_{n+r}(x) \cdots \vec{A}_{n+2}(x)), \\ &= -\det(\vec{A}_{n+r}(x) \cdots \vec{A}_{n+2}(x) \vec{A}_n(x)) - (a_{n,0} - x) \det(\vec{A}_{n+r}(x) \cdots \vec{A}_{n+1}(x)), \end{aligned}$$

so that the first two terms of (2.22) reduce to $-\prod_{\ell=n}^{n+r-1} a_{\ell,r} \det(\vec{A}_{n+r}(x) \cdots \vec{A}_{n+2}(x) \vec{A}_n(x))$. We apply this argument several times, knowing that, for $j = 1, \dots, r-1$,

$$\begin{aligned} & a_{n+r-j,r} \det(\vec{A}_{n+r+1-j}(x) \cdots \vec{A}_{n+2}(x) \vec{A}_n(x) \cdots \vec{A}_{n-j+1}(x)) \\ &= (-1)^r \det(\vec{A}_{n+r-j}(x) \cdots \vec{A}_{n+2}(x) \vec{A}_n(x) \cdots \vec{A}_{n-j}(x)) \\ &+ (-1)^{r-j} a_{n,j} \det(\vec{A}_{n+r-j}(x) \cdots \vec{A}_{n-j+1}(x)). \end{aligned}$$

Finally we obtain that the expression in (2.22) is equal to 0. This proves the lemma. \square

2.3. Generalized Christoffel–Darboux identity

For orthogonal polynomials it is known that they satisfy the Christoffel–Darboux formula; see, e.g., [9]. In [17] the authors proved a generalized Christoffel–Darboux identity for matrix orthogonality of vector polynomials. This includes a generalized Christoffel–Darboux identity for the multiple orthogonal polynomials of type I and type II in the sense that one of the vector polynomials then has just one component. Here we show that this identity can be found as a natural consequence of Section 2.2.

Theorem 2.5. *Suppose that the measures μ_1, \dots, μ_r form a weakly complete system. For the corresponding multiple orthogonal polynomials we have*

$$(x - y) \sum_{k=1}^n P_{k-1}(x) Q_{k,n}^{(i)}(y) = \gamma_n (P_n(x) P_{n-i}(y) - P_n(y) P_{n-i}(x)) \quad (2.23)$$

and

$$\sum_{k=1}^n P_{k-1}(x) Q_{k,n}^{(i)}(x) = \gamma_n (P'_n(x) P_{n-i}(x) - P_n(x) P'_{n-i}(x)), \quad (2.24)$$

$i = 1, \dots, \min(r, n)$, with $Q_{k,n}^{(i)}$ as in Definition 2.3 and γ_n as in (2.17).

Remark 2.6. The Christoffel–Darboux formulas in Theorem 2.5 are related to the generalized Christoffel–Darboux identity [17, (21)], with one vector polynomial having just 1 component. In particular, for each i , expression (2.23) is a linear combination of the vector components in [17, (21)].

Proof. Define $\vec{P}(x) = (P_0(x) \cdots P_{n-1}(x))^T$ and $\vec{Q}^{(i)}(x) = (Q_{1,n}^{(i)}(x) \cdots Q_{n,n}^{(i)}(x))^T$, $i = 1, \dots, \min(r, n)$. Eqs. (2.9) and (2.15) then reduce to

$$L_n \vec{P}(x) + P_n(x) \vec{e}_n = x \vec{P}(x) \quad (2.25)$$

and

$$\vec{Q}^{(i)}(x)^T L_n + B_n(x) \vec{e}_{n-i+1}^T = x \vec{Q}^{(i)}(x)^T. \quad (2.26)$$

Now multiply (2.25) on the right by the vector $\vec{Q}^{(i)}(y)^T$ and (2.26), evaluated at y , on the left by $\vec{P}(x)$, so that

$$\begin{aligned} L_n \vec{P}(x) \vec{Q}^{(i)}(y)^T + P_n(x) \vec{e}_n \vec{Q}^{(i)}(y)^T &= x \vec{P}(x) \vec{Q}^{(i)}(y)^T, \\ \vec{P}(x) \vec{Q}^{(i)}(y)^T L_n + B_n(y) \vec{P}(x) \vec{e}_{n-i+1}^T &= y \vec{P}(x) \vec{Q}^{(i)}(y)^T. \end{aligned}$$

Next, take the trace of these two equations and subtract. Since for two arbitrary squared matrices C and D the property $\text{tr}(CD) = \text{tr}(DC)$ holds, we then obtain

$$(x - y) \text{tr}(\vec{P}(x) \vec{Q}^{(i)}(y)^T) = P_n(x) Q_{n,n}^{(i)}(y) - B_n(y) P_{n-i}(x). \quad (2.27)$$

First of all we note that $B_n(y) = \gamma_n P_n(y)$ by Lemma 2.4. Secondly, using (2.10) and (2.11), we get

$$\begin{aligned} Q_{n,n}^{(i)}(y) &= \det(\vec{B}_n^{(1)}(y) \cdots \vec{B}_n^{(i-1)}(y) \vec{A}_n(y) \vec{B}_n^{(i+1)}(y) \cdots \vec{B}_n^{(r)}(y)) \\ &= \det \left(\underbrace{-\vec{A}_{n-1}(y) \cdots -\vec{A}_{n-i+1}(y)}_{i-1} \vec{A}_n(y) \underbrace{a_{n+r-i-1,r} \vec{A}_{n+r-i}(y) \cdots a_{n,r} \vec{A}_{n+1}(y)}_{r-i} \right) \\ &= \prod_{\ell=n}^{n+r-i-1} a_{\ell,r} (-1)^{(r-1)i} \det(\vec{A}_{n-i+r}(y) \cdots \vec{A}_{n-i+1}(y)) \\ &= (-1)^{(r-1)i} \left(\prod_{\ell=n-i}^{n-1} a_{\ell,r} \right)^{-1} B_{n-i}(y). \end{aligned}$$

Combining this with Lemma 2.4 and (2.21) we can conclude that $Q_{n,n}^{(i)}(y) = \gamma_n P_{n-i}(y)$. So, from (2.27) we finally obtain expression (2.23). If we let $y \rightarrow x$ we also find (2.24). \square

3. Multiple Gaussian quadrature

Suppose μ_1, \dots, μ_r are measures for which all the moments exist. In this section, we want to approximate a set of integrals of the kind

$$\int_{\Gamma_j} f_j(x) d\mu_j(x), \quad j = 1, \dots, r.$$

An obvious possibility is to approximate each of these integrals separately using Gaussian quadrature. However, when $f_1 = \dots = f_r = f$ we can consider to take the same set of quadrature nodes in each weighted quadrature formula. Our approximation then looks like

$$\int_{\Gamma_j} f(x) d\mu_j(x) = \sum_{\ell=1}^n w_{\ell,n}^{(j)} f(x_{\ell,n}) + E_n^{(j)}(f), \quad j = 1, \dots, r, \quad (3.1)$$

for different quadrature nodes $x_{1,n}, \dots, x_{n,n}$, which is due to Borges [5]. So, we will not necessarily have the maximal order for each of the weighted quadrature formulas. However, the advantage of this choice is that we only need n evaluations of the function f instead of rn . In accordance with the case $r = 1$, we say that the set of weighted quadrature formulas (3.1) has *vector order* $\vec{d} = (d_1, \dots, d_r) \in \mathbb{N}_0^r$ if $E_n^{(j)}(f) = 0$ for each polynomial f of degree less than or equal to d_j , $j = 1, \dots, r$.

Our goal is to maximize the vector order of (3.1) along the proper multi-indices. A necessary requirement is then that each of the quadrature formulas is interpolating, which means that we have vector order at least $(n - 1, \dots, n - 1)$. This corresponds to the conditions

$$w_{\ell,n}^{(j)} = \int_{\Gamma_j} l_{\ell,n}(x) d\mu_j(x), \quad \ell = 1, \dots, n, \quad j = 1, \dots, r, \quad (3.2)$$

where

$$l_{\ell,n}(x) = \prod_{i=1, i \neq \ell}^n \frac{x - x_{i,n}}{x_{\ell,n} - x_{i,n}}, \quad \ell = 1, \dots, n,$$

are the fundamental polynomials of Lagrange interpolation. The only freedom we still have then consists of the choice of the set of quadrature nodes. In [5], Borges already proved that the maximal vector order (along the proper multi-indices) is obtained if we choose the quadrature nodes to be the zeros of the type II multiple orthogonal polynomial P_n , corresponding to the measures μ_1, \dots, μ_r . We recall this theorem and give a proof for completeness. Of course we need that the proper multi-index \vec{v}_n is normal so that P_n is uniquely defined and has exact degree. Furthermore, we need that the zeros of P_n are simple. Note that, in the case of positive measures, these conditions are satisfied if the measures form, e.g., an AT system or Angelesco system [16,18].

Theorem 3.1 (Borges). *Suppose that the measures μ_1, \dots, μ_r form a weakly complete system and that P_n , the type II multiple orthogonal polynomial of degree n , has simple zeros. We then speak of multiple Gaussian quadrature if the weighted quadrature formulas in (3.1) are interpolating and the quadrature nodes are the zeros of P_n . In this case we have vector order $(n - 1)\vec{e} + \vec{v}_n$, where $\vec{e} = (1, \dots, 1) \in \mathbb{N}^r$. Furthermore, these quadrature formulas do not have vector order $(n - 1)\vec{e} + \vec{v}_{n+1}$.*

Proof. We prove that, with the conditions of the theorem, the j th weighted quadrature formula in (3.1) has order $n - 1 + \vec{v}_n(j)$, $j = 1, \dots, r$. Let h_j be a polynomial of degree at least n and at most $n - 1 + \vec{v}_n(j)$. (If $\vec{v}_n(j) = 0$, there is nothing to prove.) Denote by $T_{n-1}^{(j)}$ the interpolating polynomial of h_j at the zeros $x_{1,n}, \dots, x_{n,n}$ of the type II multiple orthogonal polynomial P_n . The polynomial $h_j - T_{n-1}^{(j)}$ can then be written as

$$h_j(x) - T_{n-1}^{(j)}(x) = P_n(x)R^{(j)}(x),$$

where $R^{(j)}$ is a polynomial of degree at most $\vec{v}_n(j) - 1$. Since the j th weighted quadrature formula is interpolating, we have

$$\begin{aligned} \int h_j(x) d\mu_j(x) - \sum_{\ell=1}^n h_j(x_{\ell,n}) w_{\ell,n}^{(j)} &= \int h_j(x) d\mu_j(x) - \sum_{\ell=1}^n T_{n-1}^{(j)}(x_{\ell,n}) w_{\ell,n}^{(j)} \\ &= \int (h_j(x) - T_{n-1}^{(j)}(x)) d\mu_j(x) \\ &= \int P_n(x) R^{(j)}(x) d\mu_j(x). \end{aligned}$$

By the orthogonality conditions of the type II polynomial P_n we then see that this is equal to 0.

The $x_{\ell,n}$ are the zeros of the polynomial P_n , so

$$\sum_{\ell=1}^n P_n(x_{\ell,n}) \sum_{j=1}^r A_{n+1,j}(x_{\ell,n}) w_{\ell,n}^{(j)} = 0.$$

Since \vec{v}_{n+1} is a normal index, this is different from $\int P_n(x) \sum_{j=1}^r A_{n+1,j}(x) d\mu_j(x)$, which means that we do not have vector order $(n-1)\vec{e} + \vec{v}_{n+1}$. \square

We now study the theory of multiple Gaussian quadrature from the practical point of view. In particular, we give a link with the eigenvalue problem of the banded lower Hessenberg matrix L_n ; see (2.8). First of all, from Section 2.2 we know that the zeros of the polynomial P_n are the eigenvalues of L_n . In the theorem below we show that, for multiple Gaussian quadrature, the quadrature weights can be expressed in terms of the corresponding left and right eigenvectors. This extends the expressions found in the case of Gaussian quadrature; see e.g., [10, Chapter 3, Section 2.3; 11].

Theorem 3.2. Assume that the measures μ_1, \dots, μ_r form a weakly complete system and that the type II multiple orthogonal polynomial P_n has simple zeros $x_{1,n}, \dots, x_{n,n}$. Let $\vec{v}_{\ell,n}$ be the right eigenvector of the matrix L_n corresponding to the eigenvalue $x_{\ell,n}$, with first component equal to 1. Similarly, denote by $\vec{u}_{\ell,n}$ the corresponding left eigenvector with the k_ℓ th component, the first non-zero component, equal to 1. Here $1 \leq k_\ell \leq \min(r, n)$. In the case of multiple Gaussian quadrature we then have, for $\ell = 1, \dots, n$,

$$w_{\ell,n}^{(j)} = \frac{1}{\vec{u}_{\ell,n}^T \vec{v}_{\ell,n}} \left(\sum_{k=1}^{\min(j,n)} C_{j,k} \vec{u}_{\ell,n}(k) \right), \quad j = 1, \dots, r, \quad (3.3)$$

where

$$\begin{aligned} C_{j,k} &= \int_{\Gamma_j} P_{k-1}(x) d\mu_j(x) \\ &= \sum_{i=1}^k (-1)^{k+i} m_{i-1}^{(j)} \frac{\det D_k^{(k,i)}}{\det D_{k-1}}, \quad 1 \leq k \leq j \leq r. \end{aligned} \quad (3.4)$$

Here the constants $C_{j,j}$, $j = 1, \dots, r$ are different from 0 and $w_{\ell,n}^{(j)} = 0$, $j = 1, \dots, k_\ell - 1$.

Proof. In this proof we fix $\ell \in \{1, \dots, n\}$. From Section 2.2 we know that

$$\vec{v}_{\ell,n} = (P_0(x_{\ell,n}) \cdots P_{n-1}(x_{\ell,n}))^T.$$

By Remark 2.1 we have $a_{m+r-1,r} \neq 0$, $m \geq 1$. Then it is clear that at least one of the first $\min(r, n)$ components of the left eigenvector $\vec{u}_{\ell,n}$ and at least one of the last $\min(r, n)$ components of $\vec{v}_{\ell,n}$ is different from 0. So, there exists an $i_\ell \in \{1, \dots, \min(r, n)\}$ for which $P_{n-i_\ell}(x_{\ell,n}) \neq 0$. Taking $x = x_{\ell,n}$ in (2.24) with $i = i_\ell$, we then find

$$\sum_{k=1}^n P_{k-1}(x_{\ell,n}) Q_{k,n}^{(i_\ell)}(x_{\ell,n}) = \gamma_n P'_n(x_{\ell,n}) P_{n-i_\ell}(x_{\ell,n}) \neq 0, \quad (3.5)$$

because $x_{\ell,n}$ is a simple zero of P_n . Consequently, the vector (2.16) with $i = i_\ell$ is different from $\vec{0}$ and

$$\vec{u}_{\ell,n} = \left(\underbrace{0 \cdots 0}_{k_\ell-1} \ 1 \ \frac{Q_{k_\ell+1,n}^{(i_\ell)}(x_{\ell,n})}{Q_{k_\ell,n}^{(i_\ell)}(x_{\ell,n})} \cdots \frac{Q_{n,n}^{(i_\ell)}(x_{\ell,n})}{Q_{k_\ell,n}^{(i_\ell)}(x_{\ell,n})} \right)^T. \quad (3.6)$$

Applying (3.5) we then find that

$$\vec{u}_{\ell,n}^T \vec{v}_{\ell,n} = \frac{\gamma_n P'_n(x_{\ell,n}) P_{n-i_\ell}(x_{\ell,n})}{Q_{k_\ell,n}^{(i_\ell)}(x_{\ell,n})}. \quad (3.7)$$

Next, since the weighted quadrature formulas are assumed to be interpolating, we obtain from the Christoffel–Darboux formula (2.23) with $i = i_\ell$ and $y = x_{\ell,n}$ that

$$\begin{aligned} w_{\ell,n}^{(j)} &= \int_{\Gamma_j} l_{\ell,n}(x) \, d\mu_j(x) \\ &= \frac{1}{P'_n(x_{\ell,n})} \int_{\Gamma_j} \frac{P_n(x)}{x - x_{\ell,n}} \, d\mu_j(x) \\ &= \frac{1}{\gamma_n P'_n(x_{\ell,n}) P_{n-i_\ell}(x_{\ell,n})} \sum_{k=1}^n Q_{k,n}^{(i_\ell)}(x_{\ell,n}) \int_{\Gamma_j} P_{k-1}(x) \, d\mu_j(x), \quad j = 1, \dots, r. \end{aligned}$$

Combining this with (3.7) and using orthogonality conditions of the type II polynomial P_n we then finally get

$$w_{\ell,n}^{(j)} = \frac{1}{\vec{u}_{\ell,n}^T \vec{v}_{\ell,n}} \sum_{k=1}^{\min(j,n)} \frac{Q_{k,n}^{(i_\ell)}(x_{\ell,n})}{Q_{k_\ell,n}^{(i_\ell)}(x_{\ell,n})} \int_{\Gamma_j} P_{k-1}(x) \, d\mu_j(x), \quad j = 1, \dots, r,$$

which proves (3.3). Finally we note that the proper multi-indices are normal, so we have that $C_{j,j} \neq 0$, $j = 1, \dots, r$. \square

Remark 3.3. There exists a one-to-one mapping between the sets of constants $C_{j,k} \in \mathbb{C}$, $1 \leq k \leq j \leq r$ (with $C_{j,j} \neq 0$, $1 \leq j \leq r$) and $A_{i,j} \in \mathbb{C}$, $1 \leq j \leq i \leq r$ (with $A_{j,j} \neq 0$, $1 \leq j \leq r$). By the orthogonality conditions

of the multiple orthogonal polynomials of type I and type II we obtain that

$$\begin{aligned} \sum_{j=k}^i A_{i,j} C_{j,k} &= \int P_{k-1}(x) \sum_{j=1}^i A_{i,j} d\mu_j(x) \\ &= \begin{cases} 0, & k = 1, \dots, i-1, \\ 1, & k = i, \end{cases} \quad i = 1, \dots, r. \end{aligned}$$

In particular, each of these sets can be found from the other one by solving the linear systems

$$\begin{pmatrix} C_{1,1} & C_{2,1} & \cdots & C_{i,1} \\ 0 & C_{2,2} & \cdots & C_{i,2} \\ \vdots & \ddots & \ddots & \vdots \\ 0 & \cdots & 0 & C_{i,i} \end{pmatrix} \begin{pmatrix} A_{i,1} \\ A_{i,2} \\ \vdots \\ A_{i,i} \end{pmatrix} = \begin{pmatrix} 0 \\ \vdots \\ 0 \\ 1 \end{pmatrix}, \quad i = 1, \dots, r, \quad (3.8)$$

and

$$\begin{pmatrix} A_{i,i} & 0 & \cdots & 0 \\ \vdots & \ddots & \ddots & \vdots \\ \vdots & & \ddots & 0 \\ A_{r,i} & \cdots & \cdots & A_{r,r} \end{pmatrix} \begin{pmatrix} C_{i,i} \\ C_{i+1,i} \\ \vdots \\ C_{r,i} \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix}, \quad i = 1, \dots, r, \quad (3.9)$$

respectively.

4. Conclusion

In Theorem 3.2, we proved that in the case of multiple Gaussian quadrature the quadrature nodes and weights in (3.1) can be found explicitly by solving the left and right eigenvalue problem of a banded lower Hessenberg matrix L_n . Here L_n contains the recurrence coefficients of the multiple orthogonal polynomials corresponding to the set of measures μ_1, \dots, μ_r as in (2.8). Further, we only need a set of constants $C_{j,k} \in \mathbb{C}$, $1 \leq k \leq j \leq r$ (with $C_{j,j} \neq 0$, $1 \leq j \leq r$) which can be found from the initial values of the type I multiple orthogonal polynomials by solving linear systems (3.8).

By Theorem 3.1, the weighted quadrature formulas preserve the orthogonality conditions (and normalization) for the finite set of polynomials $\bar{A}_1, \dots, \bar{A}_n$ and P_0, P_1, \dots, P_{n-1} . So, these are also the type I and type II multiple orthogonal polynomials corresponding to the set of discrete measures

$$\mu_{j,n} = \sum_{\ell=1}^n w_{\ell,n}^{(j)} \delta_{x_{\ell,n}}, \quad j = 1, \dots, r,$$

with finite support. Then note that Remark 3.3 is a nice illustration of Remark 2.2. Since we explained how to find these discrete measures starting from the recurrence coefficients and the set of initial values $A_{i,j} \in \mathbb{C}$, $1 \leq j \leq i \leq r$ (with $A_{j,j} \neq 0$, $1 \leq j \leq r$), this gives rise to a constructive proof of the spectral theorem for a finite set of multiple orthogonal polynomials. In the case of an infinite set some results for the spectral theorem were already obtained in [14,17]. However, finding necessary and sufficient conditions on the recurrence coefficients to have positive orthogonality measures on the real axis is still an open problem.

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